6-Quinolinamine, N,N,2-trimethyl-92-99-9 | DTXSID6059075

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 137 °C

Global applicability domain: Inside

Local applicability domain index: 6.58e-01

Confidence level: 3.94e-01

Nearest Neighbors from the Training Set

Image not found

Imipramine
Measured: 175
Predicted: 145

Image not found

Imipramine hydrochloride

Measured: 174 Predicted: 145 Image not found

N,N,N',N'-Tetramethylbenzidine

Measured: 194 Predicted: 153

Image not found

4,4'-Methylenebis(N,N-dimethylaniline)

Measured: 91.5 Predicted: 128 Image not found

Trimipramine
Measured: 45.0
Predicted: 119